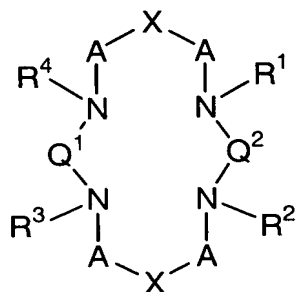
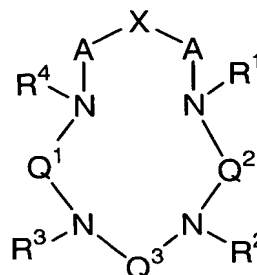


WHAT IS CLAIMED IS:

1. A compound of formulae (I) or (II):



(I)



(II)

and pharmaceutically acceptable salts thereof wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: C_1 - C_{10} alkyl substituted with 0-5 R^5 , C_2 - C_{10} alkenyl substituted with 0-5 R^5 and aryl substituted with 0-5 R^5 ;

R^5 is independently elected at each occurrence from the group: H, $C(=O)OR^{18}$, C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} , aryl substituted with 0-5 R^{13} and heterocycle substituted with 0-5 R^{13} ;

X is selected from the group: BR^6R^7 , $C(=O)$, SiR^6R^7 , GeR^6R^7 , SnR^6R^7 , NR^8 , PR^9 , $P(=O)R^9$, $P(=S)R^9$, AsR^9 and $As(=O)R^9$;

A is selected from the group: CH_2 , NR^{10} and O;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n is 2-5;

R^6 and R^7 are independently selected from the group: C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or alternatively, R^6 and R^7 may be taken together to form a transannular bridge, said bridge selected from

the group: C₃-C₁₀ alkyl substituted with 0-5 R¹³ and ortho-aryl substituted with 0-3 R¹³;

R⁸ is selected from the group: OR¹⁴, C(=O)R¹⁴, S(=O)₂R¹⁴ and P(=O)(OR¹⁴);

5 R⁹ is selected from the group: OR¹⁴, NR¹⁵R¹⁶ and CH₂NR¹⁵R¹⁶;
R¹⁰, R¹¹ and R¹² are independently selected from the group: H, C₁-C₁₀ alkyl substituted with 0-5 R¹⁷, C₂-C₁₀ alkenyl substituted with 0-5 R¹⁷ and aryl substituted with 0-3 R¹⁷;

10 R¹³ is independently selected at each occurrence from the group: H, OH, NHR¹⁸, C(=O)R¹⁸, OC(=O)R¹⁸, OC(=O)OR¹⁸, C(=O)OR¹⁸, C(=O)NR₂¹⁸, PO₃R₂¹⁸, SR¹⁸, SOR¹⁸, SO₂R¹⁸, NHC(=O)R¹⁸, NHC(=O)NHR¹⁸, CH₂OR¹⁸, CH₃ and NHC(=S)NHR¹⁸;

15 R¹⁴, R¹⁵ and R¹⁶ are independently selected from the group: hydrogen, C₁-C₁₀ alkyl substituted with 0-5 R¹³, C₂-C₁₀ alkenyl substituted with 0-5 R¹³ and aryl substituted with 0-5 R¹³;

or, alternatively, two R¹⁴ or R¹⁵ and R¹⁶ may be taken together to form a transannular bridge, said bridge
20 selected from the group: C₃-C₁₀ alkyl substituted with 0-5 R¹³ and ortho-aryl substituted with 0-3 R¹³;

R¹⁷ is independently selected at each occurrence from the group: H, OH, NHR¹⁸, C(=O)R¹⁸, OC(=O)R¹⁸, OC(=O)OR¹⁸, C(=O)OR¹⁸, C(=O)NR₂¹⁸, PO₃R₂¹⁸, SR¹⁸, SOR¹⁸, SO₂R¹⁸, NHC(=O)R¹⁸,
25 NHC(=O)NHR¹⁸ and NHC(=S)NHR¹⁸; and

R¹⁸ is independently selected at each occurrence from the group: H, C₁-C₆ alkyl, benzyl and phenyl;

with the proviso that when said compound is of formula (I) and X is P(=O)R⁹, A is not CH₂.

30

2. A compound of Claim 1, wherein:

X is selected from the group: NR⁸, PR⁹ and P(=O)R⁹;

A is CH₂;

R^8 is selected from the group: OR^{14} , $C(=O)R^{14}$ and $S(=O)_2R^{14}$; and

R^9 is $CH_2NR^{15}R^{16}$.

5 3. A compound of Claim 2 of formula (II), wherein:

X is $P(=O)OH$;

A is CH_2 ;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n is 2 or 3;

10 R^{11} and R^{12} are independently selected from the group: H, C_1-C_5 alkyl substituted with 0-3 R^{17} and aryl substituted with 0-1 R^{17} ;

15 R^{17} is independently selected at each occurrence from the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$; and

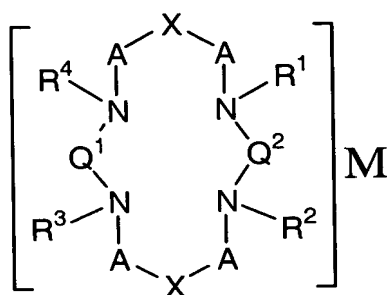
R^{18} is independently selected at each occurrence from the group: H and C_1-C_5 alkyl.

20 4. A compound of Claim 3, wherein:

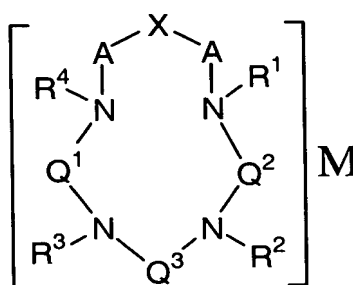
R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: H, CH_2COOH , $CH_2PO_3H_2$ and CH_2 -heterocycle substituted with 0-3 R^{13} ; and

25 R^{13} is independently selected at each occurrence from the group: H, OH, NH_2 , COOH, PO_3H_2 , CH_2OH , CH_3 and SO_3H .

5. A radiopharmaceutical of formulae (III) or (IV):



(III)



(IV)

and pharmaceutically acceptable salts thereof, wherein:

M is selected from the group: ^{64}Cu , ^{67}Cu , ^{67}Ga , ^{68}Ga , $^{99\text{m}}\text{Tc}$, ^{111}In , ^{90}Y , ^{149}Pr , ^{153}Sm , ^{159}Gd , ^{166}Ho , ^{169}Yb , ^{177}Lu , ^{186}Re and ^{188}Re ;

R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from: $\text{C}_1\text{-C}_{10}$ alkyl substituted with 0-5 R^5 , $\text{C}_2\text{-C}_{10}$ alkenyl substituted with 0-5 R^5 and aryl substituted with 0-5 R^5 ;

R^5 is independently elected at each occurrence from: H, $\text{C}(=\text{O})\text{OR}^{18}$, $\text{C}(=\text{O})\text{OR}^{23}$, $\text{C}_1\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} , $\text{C}_2\text{-C}_{10}$ alkenyl substituted with 0-5 R^{13} , aryl substituted with 0-5 R^{13} and heterocycle substituted with 0-5 R^{13} ;

X is selected from the group: BR^6R^7 , $\text{C}(=\text{O})$, SiR^6R^7 , GeR^6R^7 , SnR^6R^7 , NR^8 , PR^9 , $\text{P}(=\text{O})\text{R}^9$, $\text{P}(=\text{S})\text{R}^9$, AsR^9 and $\text{As}(=\text{O})\text{R}^9$;

A is selected from the group: CH_2 , NR^{10} and O;

Q^1 , Q^2 , and Q^3 are independently $-(\text{CR}^{11}\text{R}^{12})_n-$, wherein: n is 2-5;

R^6 and R^7 are independently selected from the group: $\text{C}_1\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} , $\text{C}_2\text{-C}_{10}$ alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or alternatively, R^6 and R^7 may be taken together to form a transannular bridge, said bridge selected from the group: $\text{C}_3\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$, $S(=O)_2R^{14}$ and $P(=O)(OR^{14})$;

R^9 is selected from the group: OR^{14} , $NR^{15}R^{16}$ and $CH_2NR^{15}R^{16}$;

5 R^{10} , R^{11} and R^{12} are independently selected from the group: H, C_1-C_{10} alkyl substituted with 0-5 R^{17} , C_2-C_{10} alkenyl substituted with 0-5 R^{17} and aryl substituted with 0-3 R^{17} ;

10 R^{13} is independently selected at each occurrence from the group: H, OH, OR^{23} , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $OC(=O)OR^{23}$, $C(=O)OR^{18}$, $C(=O)OR^{23}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, $PO_3R^{18}R^{23}$, SR^{18} , SR^{23} , SOR^{18} , SO_2R^{18} , SOR^{23} , SO_2R^{23} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$, CH_2OR^{18} , CH_2OR^{23} , CH_3 and $NHC(=S)NHR^{18}$;

15 R^{14} , R^{15} and R^{16} are independently selected from the group: C_1-C_{10} alkyl substituted with 0-5 R^{13} , C_2-C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

20 or, alternatively, two R^{14} or R^{15} and R^{16} may be taken together to form a transannular bridge, said bridge selected from the group: C_3-C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

25 R^{17} is independently selected at each occurrence from the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SR^{18} , SOR^{18} , SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$;

R^{18} is independently selected at each occurrence from the group: H, C_1-C_6 alkyl, benzyl and phenyl; and

R^{23} is a bond to the metal M;

30 with the proviso that when said radiopharmaceutical is of formula (III) and X is $P(=O)R^9$, A is not CH_2 .

6. A radiopharmaceutical of Claim 5, wherein:

X is selected from the group: NR^8 , PR^9 and $P(=O)R^9$;

A is CH_2 ;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$ and $S(=O)_2R^{14}$; and

R^9 is $CH_2NR^{15}R^{16}$.

5 7. A radiopharmaceutical of Claim 6 of formula (IV),
wherein:

X is $P(=O)OH$;

A is CH_2 ;

10 Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n
is 2 or 3;

R^{11} and R^{12} are independently selected from the group: H,
 C_1-C_5 alkyl substituted with 0-3 R^{17} and aryl substituted
with 0-1 R^{17} ;

15 R^{17} is independently selected at each occurrence from
the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$,
 $C(=O)OR^{18}$, $C(=O)NR^{18}_2$, $PO_3R^{18}_2$, SO_2R^{18} , $NHC(=O)R^{18}$,
 $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$; and

R^{18} is independently selected at each occurrence from
the group: H and C_1-C_3 alkyl.

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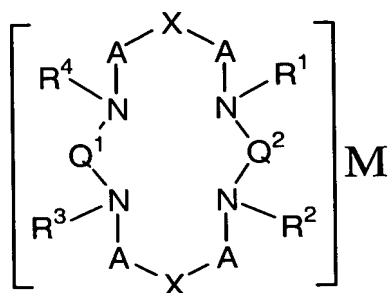
8. A radiopharmaceutical of Claim 7, wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each
occurrence from the group: H, CH_2COOH , $CH_2PO_3H_2$ and CH_2 -
heterocycle substituted with 0-3 R^{13} ; and

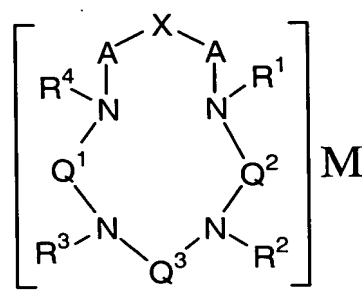
25 R^{13} is independently selected at each occurrence from
the group: H, OR^{23} , $OC(=O)OR^{23}$, $C(=O)OR^{23}$, $PO_3R^{18}R^{23}$, SR^{23} ,
 SOR^{23} , SO_2R^{23} , CH_2OR^{23} , OH, NH_2 , COOH, PO_3H_2 , CH_2OH , CH_3 and
 SO_3H .

30

9. A MRI contrast agent of the formulae (V) or (VI):



(V)



(VI)

and pharmaceutically acceptable salts thereof, wherein:

M is a paramagnetic metal ion of atomic number selected from the group: 21-29, 42-44 and 58-70;

R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from: C_1 - C_{10} alkyl substituted with 0-5 R^5 , C_2 - C_{10} alkenyl substituted with 0-5 R^5 and aryl substituted with 0-5 R^5 ;

R^5 is independently elected at each occurrence from: H, $C(=O)OR^{18}$, $C(=O)OR^{23}$, C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} , aryl substituted with 0-5 R^{13} and heterocycle substituted with 0-5 R^{13} ;

X is selected from the group: BR^6R^7 , $C(=O)$, SiR^6R^7 , GeR^6R^7 , SnR^6R^7 , NR^8 , PR^9 , $P(=O)R^9$, $P(=S)R^9$, AsR^9 and $As(=O)R^9$;

A is selected from the group: CH_2 , NR^{10} and O;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n is 2-5;

R^6 and R^7 are independently selected from the group: C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or alternatively, R^6 and R^7 may be taken together to form a transannular bridge, said bridge selected from the group: C_3 - C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$, $S(=O)_2R^{14}$ and $P(=O)(OR^{14})$;

R^9 is selected from the group: OR^{14} , $NR^{15}R^{16}$ and $CH_2NR^{15}R^{16}$;

5 R^{10} , R^{11} and R^{12} are independently selected from the group: H, C_1-C_{10} alkyl substituted with 0-5 R^{17} , C_2-C_{10} alkenyl substituted with 0-5 R^{17} and aryl substituted with 0-3 R^{17} ;

10 R^{13} is independently selected at each occurrence from the group: H, OH, OR^{23} , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $OC(=O)OR^{23}$, $C(=O)OR^{18}$, $C(=O)OR^{23}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, $PO_3R^{18}R^{23}$, SR^{18} , SR^{23} , SOR^{18} , SO_2R^{18} , SOR^{23} , SO_2R^{23} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$, CH_2OR^{18} , CH_2OR^{23} , CH_3 and $NHC(=S)NHR^{18}$;

15 R^{14} , R^{15} and R^{16} are independently selected from the group: C_1-C_{10} alkyl substituted with 0-5 R^{13} , C_2-C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

20 or, alternatively, two R^{14} or R^{15} and R^{16} may be taken together to form a transannular bridge, said bridge selected from the group: C_3-C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

25 R^{17} is independently selected at each occurrence from the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SR^{18} , SOR^{18} , SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$;

R^{18} is independently selected at each occurrence from the group: H, C_1-C_6 alkyl, benzyl and phenyl; and

R^{23} is a bond to the metal M;

30 with the proviso that when said MRI contrast agent is of formula (V) and X is $P(=O)R^9$, A is not CH_2 .

10. A MRI contrast agent of Claim 9, wherein:

X is selected from the group: NR^8 , PR^9 and $P(=O)R^9$;

A is CH_2 ;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$ and $S(=O)_2R^{14}$; and

R^9 is $CH_2NR^{15}R^{16}$.

5 11. A MRI contrast agent of Claim 10 of formula (VI),
wherein:

X is $P(=O)OH$;

A is CH_2 ;

10 Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n
is 2 or 3;

R^{11} and R^{12} are independently selected from the group:
 H , C_1-C_5 alkyl substituted with 0-3 R^{17} and aryl
substituted with 0-1 R^{17} ;

15 R^{17} is independently selected at each occurrence from
the group: H , OH , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$,
 $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SO_2R^{18} , $NHC(=O)R^{18}$,
 $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$; and

R^{18} is independently selected at each occurrence from
the group: H and C_1-C_3 alkyl.

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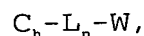
12. A MRI contrast agent of Claim 11, wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each
occurrence from the group: H , CH_2COOH , $CH_2PO_3H_2$ and CH_2 -
heterocycle substituted with 0-3 R^{13} ; and

25 R^{13} is independently selected at each occurrence from
the group: H , OR^{23} , $OC(=O)OR^{23}$, $C(=O)OR^{23}$, $PO_3R^{18}R^{23}$, SR^{23} ,
 SOR^{23} , SO_2R^{23} , CH_2OR^{23} , OH , NH_2 , $COOH$, PO_3H_2 , CH_2OH , CH_3 and
 SO_3H .

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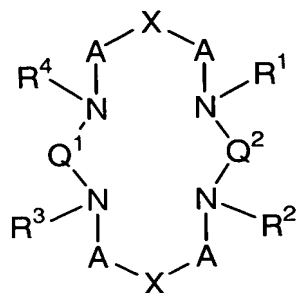
13. A conjugate of the formula:



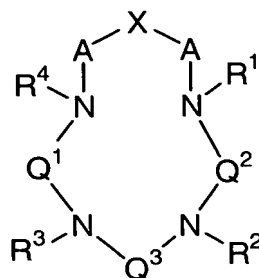
and pharmaceutically acceptable salts thereof,

wherein:

C_n is a chelator of formulae (VII) or (VIII):



(VII)



(VIII)

wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: C_1 - C_{10} alkyl substituted with 0-5 R^5 , C_2 - C_{10} alkenyl substituted with 0-5 R^5 and aryl substituted with 0-5 R^5 ;

R^5 is independently elected at each occurrence from the group: H, $C(=O)OR^{18}$, C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} , aryl substituted with 0-5 R^{13} and heterocycle substituted with 0-5 R^{13} ;

X is selected from the group: BR^6R^7 , $C(=O)$, SiR^6R^7 , GeR^6R^7 , SnR^6R^7 , NR^8 , PR^9 , $P(=O)R^9$, $P(=S)R^9$, AsR^9 and $As(=O)R^9$;

A is selected from the group: CH_2 , NR^{10} and O;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n is 2-5;

R^6 and R^7 are independently selected from the group: C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or alternatively, R^6 and R^7 may be taken together to form a transannular bridge, said bridge selected from

the group: C_3-C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

R^8 is selected from the group: OR^{14} , $C(=O)R^{14}$, $S(=O)_2R^{14}$ and $P(=O)(OR^{14})$;

5 R^9 is selected from the group: OR^{14} , $NR^{15}R^{16}$ and $CH_2NR^{15}R^{16}$;
 R^{10} , R^{11} and R^{12} are independently selected from the group: H , C_1-C_{10} alkyl substituted with 0-5 R^{17} , C_2-C_{10} alkenyl substituted with 0-5 R^{17} and aryl substituted with 0-3 R^{17} ;

10 R^{13} is independently selected at each occurrence from the group: H , OH , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SR^{18} , SOR^{18} , SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$, CH_2OR^{18} , CH_3 , $NHC(=S)NHR^{18}$ and a bond to L_n ;

15 R^{14} , R^{15} and R^{16} are independently selected from the group: hydrogen, C_1-C_{10} alkyl substituted with 0-5 R^{13} , C_2-C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or, alternatively, two R^{14} or R^{15} and R^{16} may be taken together to form a transannular bridge, said bridge
 20 selected from the group: C_3-C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

R^{17} is independently selected at each occurrence from the group: H , OH , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SR^{18} , SOR^{18} , SO_2R^{18} , $NHC(=O)R^{18}$,
 25 $NHC(=O)NHR^{18}$, $NHC(=S)NHR^{18}$ and a bond to L_n ;

R^{18} is independently selected at each occurrence from the group: H , C_1-C_6 alkyl, benzyl, phenyl and a bond to L_n ;

L_n is a linking group of formula:

30
$$L^1 - [Y^1(CR^{19}R^{20})_f(Z^1)_fY^2]_f - L^2,$$

wherein:

L^1 is $-(CH_2)_gZ^1]_g - (CR^{19}R^{20})_g -$;

L^2 is $-(CR^{19}R^{20})_g - [Z^1(CH_2)_g]_g -$;

g is independently 0-10;

g' is independently 0-1;

g" is independently 0-10;

f is independently 0-10;

5 f' is independently 0-10;

f" is independently 0-1;

Y¹ and Y², at each occurrence, are independently selected from the group: a bond, O, NR²⁰, C=O, C(=O)O, OC(=O)O, C(=O)NH-, C=NR²⁰, S, SO, SO₂, NHC(=O),
10 (NH)₂C(=O) and (NH)₂C=S;

R¹⁹ and R²⁰ are independently selected at each occurrence from the group: H, C₁-C₁₀ alkyl substituted with 0-5 R²¹ and alkaryl wherein the aryl is substituted with 0-5 R²¹;
R²¹;

15 R²¹ is independently selected at each occurrence from the group: NHR²², C(=O)R²², OC(=O)R²², OC(=O)OR²², C(=O)OR²², C(=O)NR₂²², -CN, SR²², SOR²², SO₂R²², NHC(=O)R²², NHC(=O)NHR²², NHC(=S)NHR²² and a bond to W;

20 R²² is independently selected at each occurrence from the group: H, C₁-C₆ alkyl, benzyl, phenyl and a bond to W; and

W is a biologically active molecule selected from the group: IIb/IIIa receptor ligands, fibrin binding peptides, leukocyte binding peptides, chemotactic
25 peptides, somatostatin analogs, selectin binding peptides, vitronectin receptor antagonists and tyrosine kinase inhibitors;

with the proviso that when said chelator is of formula (VII) and X is P(=O)R⁹, A is not CH₂.

30

14. A conjugate of Claim 13, wherein:

X is selected from the group: NR⁸, PR⁹ and P(=O)R⁹;

A is CH₂;

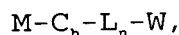
- R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$ and $S(=O)_2R^{14}$;
 R^9 is $CH_2NR^{15}R^{16}$;
 g is independently 0-5;
5 g'' is independently 0-5;
 f is independently 0-5;
 f' is independently 0-5;
 Y^1 and Y^2 , at each occurrence, are independently selected from the group: a bond, O, NR^{20} , $C=O$, $C(=O)O$,
10 $OC(=O)O$, $C(=O)NH-$, SO , SO_2 , $NHC(=O)$, $(NH)_2C(=O)$ and $(NH)_2C=S$; and
 R^{21} is independently selected at each occurrence from the group: NHR^{22} , $C(=O)R^{22}$, $OC(=O)R^{22}$, $OC(=O)OR^{22}$, $C(=O)OR^{22}$, $C(=O)NR^{22}_2$, SO_2R^{22} , $NHC(=O)R^{22}$, $NHC(=O)NHR^{22}$,
15 $NHC(=S)NHR^{22}$ and a bond to W.
15. A conjugate of Claim 14 wherein:
Ch is a chelator of formula (VIII);
X is $P(=O)OH$;
20 A is CH_2 ;
 Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n is 2 or 3;
 R^{11} and R^{12} are independently selected from the group: H, C_1-C_5 alkyl substituted with 0-3 R^{17} and aryl substituted with 0-1 R^{17} ;
25 R^{17} is independently selected at each occurrence from the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR^{18}_2$, $PO_3R^{18}_2$, SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$; and
30 R^{18} is independently selected at each occurrence from the group: H and C_1-C_5 alkyl.

16. A conjugate of Claim 15, wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: H, CH_2COOH , $\text{CH}_2\text{PO}_3\text{H}_2$ and CH_2 -heterocycle substituted with 0-3 R^{13} ; and

5 R^{13} is independently selected at each occurrence from the group: H, OH, NH_2 , COOH, PO_3H_2 , CH_2OH , CH_3 and SO_3H .

17. A radiopharmaceutical of the formula:



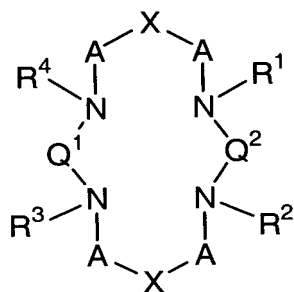
10 and pharmaceutically acceptable salts thereof,

wherein,

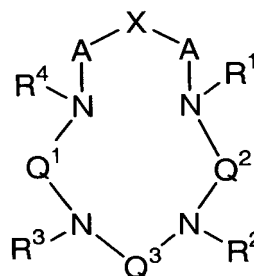
M is selected from the group: ^{64}Cu , ^{67}Cu , ^{67}Ga , ^{68}Ga , $^{99\text{m}}\text{Tc}$, ^{111}In , ^{90}Y , ^{149}Pr , ^{153}Sm , ^{159}Gd , ^{166}Ho , ^{169}Yb , ^{177}Lu , ^{186}Re and ^{188}Re ;

C_n is a chelator of formulae (IX) or (X):

15



(IX)



(X)

wherein:

20 R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: C_1 - C_{10} alkyl substituted with 0-5 R^5 , C_2 - C_{10} alkenyl substituted with 0-5 R^5 and aryl substituted with 0-5 R^5 ;

25 R^5 is independently elected at each occurrence from the group: H, $\text{C}(=\text{O})\text{OR}^{18}$, $\text{C}(=\text{O})\text{OR}^{23}$, C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} , aryl substituted with 0-5 R^{13} and heterocycle substituted with 0-5 R^{13} ;

X is selected from the group: BR^6R^7 , $\text{C}(=\text{O})$, SiR^6R^7 , GeR^6R^7 , SnR^6R^7 , NR^8 , PR^9 , $\text{P}(=\text{O})\text{R}^9$, $\text{P}(=\text{S})\text{R}^9$, AsR^9 and $\text{As}(=\text{O})\text{R}^9$;

A is selected from the group: CH_2 , NR^{10} and O;

5 Q^1 , Q^2 , and Q^3 are independently $-(\text{CR}^{11}\text{R}^{12})_n-$, wherein: n is 2-5;

R^6 and R^7 are independently selected from the group: $\text{C}_1\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} , $\text{C}_2\text{-C}_{10}$ alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or alternatively, R^6 and R^7 may be taken together to form a transannular bridge, said bridge selected from the group: $\text{C}_3\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

15 R^8 is selected from the group: OR^{23} , OR^{14} , $\text{C}(=\text{O})\text{R}^{14}$, $\text{S}(=\text{O})_2\text{R}^{14}$ and $\text{P}(=\text{O})(\text{OR}^{14})$;

R^9 is selected from the group: OR^{14} , $\text{NR}^{15}\text{R}^{16}$ and $\text{CH}_2\text{NR}^{15}\text{R}^{16}$;

R^{10} , R^{11} and R^{12} are independently selected from the group: H, $\text{C}_1\text{-C}_{10}$ alkyl substituted with 0-5 R^{17} , $\text{C}_2\text{-C}_{10}$ alkenyl substituted with 0-5 R^{17} and aryl substituted with 0-3 R^{17} ;

R^{13} is independently selected at each occurrence from the group: H, OH, OR^{23} , NHR^{18} , $\text{C}(=\text{O})\text{R}^{18}$, $\text{OC}(=\text{O})\text{OR}^{23}$, $\text{OC}(=\text{O})\text{R}^{18}$, $\text{C}(=\text{O})\text{OR}^{23}$, $\text{OC}(=\text{O})\text{OR}^{18}$, $\text{C}(=\text{O})\text{OR}^{18}$, $\text{C}(=\text{O})\text{NR}_2^{18}$, $\text{PO}_3\text{R}_2^{18}$, $\text{PO}_3\text{R}^{18}\text{R}^{23}$, SR^{18} , SR^{23} , SOR^{18} , SO_2R^{18} , SOR^{23} , SO_2R^{23} , $\text{NHC}(=\text{O})\text{R}^{18}$, $\text{NHC}(=\text{O})\text{NHR}^{18}$, $\text{CH}_2\text{OR}^{18}$, $\text{CH}_2\text{OR}^{23}$, CH_3 , $\text{NHC}(=\text{S})\text{NHR}^{18}$ and a bond to L_n ;

R^{14} , R^{15} and R^{16} are independently selected from the group: $\text{C}_1\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} , $\text{C}_2\text{-C}_{10}$ alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

or, alternatively, two R^{14} or R^{15} and R^{16} may be taken together to form a transannular bridge, said bridge selected from the group: $\text{C}_3\text{-C}_{10}$ alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

R^{17} is independently selected at each occurrence from the group: H , OH , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SR^{18} , SOR^{18} , SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$, $NHC(=S)NHR^{18}$ and a bond to L_n ;

5 R^{18} is independently selected at each occurrence from the group: H , C_1 - C_6 alkyl, benzyl, phenyl and a bond to L_n ;

R^{23} is a bond to the metal M ;

L_n is a linking group of formula:

10
$$L^1 - [Y^1 (CR^{19} R^{20})_f (Z^1)_{f'} Y^2]_{f''} - L^2,$$

wherein:

L^1 is $-(CH_2)_g Z^1]_{g'} - (CR^{19} R^{20})_{g''} -$;

L^2 is $-(CR^{19} R^{20})_{g''} - [Z^1 (CH_2)_g]_{g'} -$;

g is independently 0-10;

15 g' is independently 0-1;

g'' is independently 0-10;

f is independently 0-10;

f' is independently 0-10;

f'' is independently 0-1;

20 Y^1 and Y^2 , at each occurrence, are independently selected from the group: a bond, O , NR^{20} , $C=O$, $C(=O)O$, $OC(=O)O$, $C(=O)NH-$, $C=NR^{20}$, S , SO , SO_2 , $NHC(=O)$, $(NH)_2C(=O)$ and $(NH)_2C=S$;

25 R^{19} and R^{20} are independently selected at each occurrence from the group: H , C_1 - C_{10} alkyl substituted with 0-5 R^{21} and alkaryl wherein the aryl is substituted with 0-5 R^{21} ;

30 R^{21} is independently selected at each occurrence from the group: NHR^{22} , $C(=O)R^{22}$, $OC(=O)R^{22}$, $OC(=O)OR^{22}$, $C(=O)OR^{22}$, $C(=O)NR_2^{22}$, $-CN$, SR^{22} , SOR^{22} , SO_2R^{22} , $NHC(=O)R^{22}$, $NHC(=O)NHR^{22}$, $NHC(=S)NHR^{22}$ and a bond to W ;

R^{22} is independently selected at each occurrence from the group: H, C_1-C_6 alkyl, benzyl, phenyl and a bond to W; and

W is a biologically active molecule selected from the group: IIB/IIIA receptor ligands, fibrin binding peptides, leukocyte binding peptides, chemotactic peptides, somatostatin analogs, selectin binding peptides, vitronectin receptor antagonists and tyrosine kinase inhibitors;

with the proviso that when said chelator is of formula (IX) and X is $P(=O)R^9$, A is not CH_2 .

18. A radiopharmaceutical of Claim 17, wherein:

X is selected from the group: NR^8 , PR^9 and $P(=O)R^9$;

A is CH_2 ;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$ and $S(=O)_2R^{14}$;

R^9 is $CH_2NR^{15}R^{16}$;

g is independently 0-5;

g" is independently 0-5;

f is independently 0-5;

f' is independently 0-5;

Y^1 and Y^2 , at each occurrence, are independently selected from the group: a bond, O, NR^{20} , C=O, $C(=O)O$, $OC(=O)O$, $C(=O)NH-$, SO, SO_2 , $NHC(=O)$, $(NH)_2C(=O)$ and $(NH)_2C=S$; and

R^{21} is independently selected at each occurrence from the group: NHR^{22} , $C(=O)R^{22}$, $OC(=O)R^{22}$, $OC(=O)OR^{22}$, $C(=O)OR^{22}$, $C(=O)NR^{22}$, SO_2R^{22} , $NHC(=O)R^{22}$, $NHC(=O)NHR^{22}$, $NHC(=S)NHR^{22}$ and a bond to W.

19. A radiopharmaceutical of Claim 18, wherein:

Ch is a chelator of formula (X);

X is $P(=O)OH$;

A is CH_2 ;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n
5 is 2 or 3;

R^{11} and R^{12} are independently selected from the group:
H, C_1-C_5 alkyl substituted with 0-3 R^{17} and aryl
substituted with 0-1 R^{17} ;

10 R^{17} is independently selected at each occurrence from
the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$,
 $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SO_2R^{18} , $NHC(=O)R^{18}$,
 $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$; and

R^{18} is independently selected at each occurrence from
the group: H and C_1-C_3 alkyl.

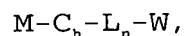
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20. A radiopharmaceutical of Claim 19, wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each
occurrence from the group: H, CH_2COOH , $CH_2PO_3H_2$ and CH_2 -
heterocycle substituted with 0-3 R^{13} ; and

20 R^{13} is independently selected at each occurrence from
the group: H, OR^{23} , $OC(=O)OR^{23}$, $C(=O)OR^{23}$, $PO_3R^{18}R^{23}$, SR^{23} ,
 SOR^{23} , SO_2R^{23} , CH_2OR^{23} , OH, NH_2 , COOH, PO_3H_2 , CH_2OH , CH₃ and
 SO_3H .

25 21. A MRI contrast agent of the formula:

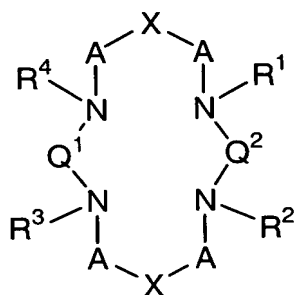


and pharmaceutically acceptable salt thereof,

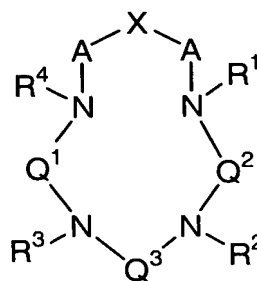
wherein:

30 M is a paramagnetic metal ion of atomic number selected
from the group: 21-29, 42-44 and 58-70;

C_h is a chelator of formulae (XI) or (XII):



(XI)



(XII)

wherein:

5 R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: C_1 - C_{10} alkyl substituted with 0-5 R^5 , C_2 - C_{10} alkenyl substituted with 0-5 R^5 and aryl substituted with 0-5 R^5 ;

10 R^5 is independently elected at each occurrence from the group: H, $C(=O)OR^{18}$, $C(=O)OR^{23}$, C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} , aryl substituted with 0-5 R^{13} and heterocycle substituted with 0-5 R^{13} ;

15 X is selected from the group: BR^6R^7 , $C(=O)$, SiR^6R^7 , GeR^6R^7 , SnR^6R^7 , NR^8 , PR^9 , $P(=O)R^9$, $P(=S)R^9$, AsR^9 and $As(=O)R^9$;

A is selected from the group: CH_2 , NR^{10} and O;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein: n is 2-5;

20 R^6 and R^7 are independently selected from the group: C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

25 or alternatively, R^6 and R^7 may be taken together to form a transannular bridge, said bridge selected from the group: C_3 - C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$, $S(=O)_2R^{14}$ and $P(=O)(OR^{14})$;

R^9 is selected from the group: OR^{14} , $NR^{15}R^{16}$ and $CH_2NR^{15}R^{16}$;

R^{10} , R^{11} and R^{12} are independently selected from the group: H, C_1 - C_{10} alkyl substituted with 0-5 R^{17} , C_2 - C_{10} alkenyl substituted with 0-5 R^{17} and aryl substituted with 0-3 R^{17} ;

5 R^{13} is independently selected at each occurrence from the group: H, OH, OR^{23} , NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $OC(=O)OR^{23}$, $C(=O)OR^{18}$, $C(=O)OR^{23}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, $PO_3R^{18}R^{23}$, SR^{18} , SR^{23} , SOR^{18} , SO_2R^{18} , SOR^{23} , SO_2R^{23} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$, CH_2OR^{18} , CH_2OR^{23} , CH_3 , $NHC(=S)NHR^{18}$
10 and a bond to L_n ;

R^{14} , R^{15} and R^{16} are independently selected from the group: C_1 - C_{10} alkyl substituted with 0-5 R^{13} , C_2 - C_{10} alkenyl substituted with 0-5 R^{13} and aryl substituted with 0-5 R^{13} ;

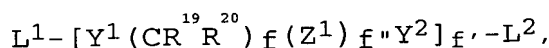
15 or, alternatively, two R^{14} or R^{15} and R^{16} may be taken together to form a transannular bridge, said bridge selected from the group: C_3 - C_{10} alkyl substituted with 0-5 R^{13} and ortho-aryl substituted with 0-3 R^{13} ;

20 R^{17} is independently selected at each occurrence from the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR_2^{18}$, $PO_3R_2^{18}$, SR^{18} , SOR^{18} , SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$, $NHC(=S)NHR^{18}$ and a bond to L_n ;

25 R^{18} is independently selected at each occurrence from the group: H, C_1 - C_6 alkyl, benzyl, phenyl and a bond to L_n ;

R^{23} is a bond to the metal M;

L_n is a linking group of formula:



30

wherein:

L^1 is $-(CH_2)_g Z^1]_g - (CR^{19}R^{20})_g -$;

L^2 is $-(CR^{19}R^{20})_g - [Z^1 (CH_2)_g]_g -$;

g is independently 0-10;

g' is independently 0-1;

g" is independently 0-10;

f is independently 0-10;

5 f' is independently 0-10;

f" is independently 0-1;

Y¹ and Y², at each occurrence, are independently selected from the group: a bond, O, NR²⁰, C=O, C(=O)O, OC(=O)O, C(=O)NH-, C=NR²⁰, S, SO, SO₂, NHC(=O),
10 (NH)₂C(=O) and (NH)₂C=S;

R¹⁹ and R²⁰ are independently selected at each occurrence from: H, C₁-C₁₀ alkyl substituted with 0-5 R²¹ and alkaryl wherein the aryl is substituted with 0-5 R²¹;

15 R²¹ is independently selected at each occurrence from the group: NHR²², C(=O)R²², OC(=O)R²², OC(=O)OR²², C(=O)OR²², C(=O)NR₂²², -CN, SR²², SOR²², SO₂R²², NHC(=O)R²², NHC(=O)NHR²², NHC(=S)NHR²² and a bond to W;

20 R²² is independently selected at each occurrence from the group: H, C₁-C₆ alkyl, benzyl, phenyl and a bond to W; and

25 W is a biologically active molecule selected from the group: IIb/IIIa receptor ligands, fibrin binding peptides, leukocyte binding peptides, chemotactic peptides, somatostatin analogs, selectin binding peptides, vitronectin receptor antagonists and tyrosine kinase inhibitors

with the proviso that when said chelator is of formula (XI) and X is P(=O)R⁹, A is not CH₂.

30 22. A MRI contrast agent of Claim 21, wherein:

X is selected from the group: NR⁸, PR⁹ and P(=O)R⁹;

A is CH₂;

R^8 is selected from the group: OR^{23} , OR^{14} , $C(=O)R^{14}$ and $S(=O)_2R^{14}$;

R^9 is $CH_2NR^{15}R^{16}$;

g is independently 0-5;

5 g'' is independently 0-5;

f is independently 0-5;

f' is independently 0-5;

10 Y^1 and Y^2 , at each occurrence, are independently selected from the group: a bond, O, NR^{20} , $C=O$, $C(=O)O$, $OC(=O)O$; $C(=O)NH-$, SO , SO_2 , $NHC(=O)$, $(NH)_2C(=O)$ and $(NH)_2C=S$; and

15 R^{21} is independently selected at each occurrence from the group selected from the group: NHR^{22} , $C(=O)R^{22}$, $OC(=O)R^{22}$, $OC(=O)OR^{22}$, $C(=O)OR^{22}$, $C(=O)NR^{22}_2$, SO_2R^{22} , $NHC(=O)R^{22}$, $NHC(=O)NHR^{22}$, $NHC(=S)NHR^{22}$ and a bond to W.

23. A MRI contrast agent of Claim 22, wherein:

Ch is a chelator of formula (XII);

X is $P(=O)OH$;

20 A is CH_2 ;

Q^1 , Q^2 , and Q^3 are independently $-(CR^{11}R^{12})_n-$, wherein n is 2 or 3;

25 R^{11} and R^{12} are independently chosen from the group: H, C_1-C_5 alkyl substituted with 0-3 R^{17} and aryl substituted with 0-1 R^{17} ;

R^{17} is independently selected at each occurrence from the group: H, OH, NHR^{18} , $C(=O)R^{18}$, $OC(=O)R^{18}$, $OC(=O)OR^{18}$, $C(=O)OR^{18}$, $C(=O)NR^{18}_2$, $PO_3R^{18}_2$, SO_2R^{18} , $NHC(=O)R^{18}$, $NHC(=O)NHR^{18}$ and $NHC(=S)NHR^{18}$; and

30 R^{18} is independently selected at each occurrence from the group: H and C_1-C_3 alkyl.

24. A MRI contrast agent of Claim 23, wherein:

R^1 , R^2 , R^3 and R^4 are independently selected at each occurrence from the group: H, CH_2COOH , $\text{CH}_2\text{PO}_3\text{H}_2$, CH_2 -heterocycle substituted with 0-3 R^{13} ; and

5 R^{13} is independently selected at each occurrence from the group: H, OR^{23} , $\text{OC}(=\text{O})\text{OR}^{23}$, $\text{C}(=\text{O})\text{OR}^{23}$, $\text{PO}_3\text{R}^{18}\text{R}^{23}$, SR^{23} , SOR^{23} , SO_2R^{23} , $\text{CH}_2\text{OR}^{23}$, OH, NH_2 , COOH, PO_3H_2 , CH_2OH , CH₃ and SO_3H .

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